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Acyl Chloride

An acyl chloride (or acid chloride) is an organic compound with the functional group -CO-Cl. Their formula is usually written RCOCl, where R is a side chain. They are usually considered to be reactive derivatives of carboxylic acids. A specific example of an acyl chloride is acetyl chloride, CH_3COCl. Acyl chlorides are the most important subset of acyl halides, e.g. acetyl bromide.

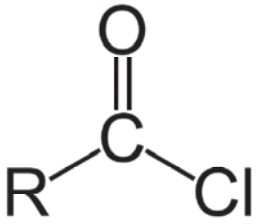


Figure: *General chemical structure of an acyl chloride*

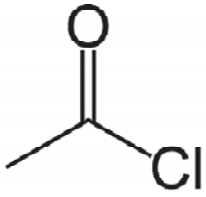


Figure: *Example of an acyl chloride: acetyl chloride or ethanoyl chloride*

Properties

Lacking the ability to form hydrogen bonds, acid chlorides have lower boiling and melting points than similar carboxylic acids. For example, acetic

acid boils at 118 °C, whereas acetyl chloride boils at 51 °C. Like most carbonyl compounds, infrared spectroscopy reveals a band near 1750 cm^{-1}.

Synthesis

Industrial Routes

The industrial route to acetyl chloride involves the reaction of acetic anhydride with hydrogen chloride. For benzoyl chloride, the partial hydrolysis of benzotrichloride is useful:

$$C_6H_5CCl_3 + H_2O \rightarrow C_6H_5C(O)Cl + 2HCl$$

Laboratory Methods

In the laboratory, acyl chlorides are generally prepared in the same manner as alkyl chlorides, by replacing the corresponding hydroxy substituents with chlorides.

Thus, carboxylic acids are treated with thionyl chloride ($SOCl_2$), phosphorus trichloride (PCl_3), or phosphorus pentachloride (PCl_5):

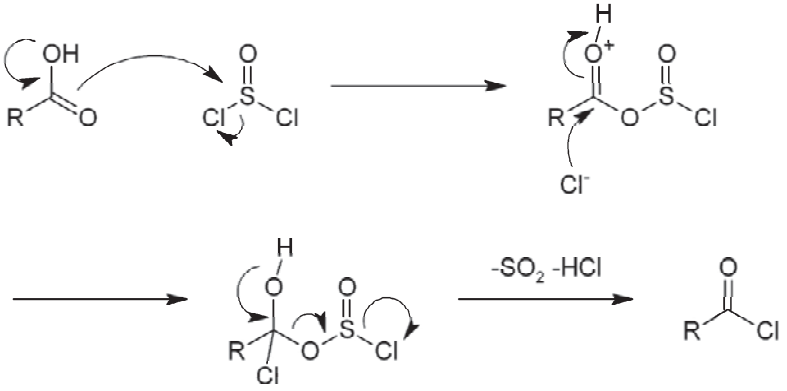
$$RCOOH + SOCl_2 \rightarrow RCOCl + SO_2 + HCl$$

$$3\ RCOOH + PCl_3 \rightarrow 3\ RCOCl + H_3PO_3$$

$$RCOOH + PCl_5 \rightarrow RCOCl + POCl_3 + HCl$$

The reaction with thionyl chloride may be catalysed by dimethylformamide. In this reaction, the sulfur dioxide (SO_2) and hydrogen chloride (HCl) generated are both gases that can leave the reaction vessel, driving the reaction forward.

Excess thionyl chloride (b.p. 79 °C) is easily evaporated as well. The reaction mechanisms involving thionyl chloride and phosphorus pentachloride are similar; the mechanism with thionyl chloride is illustrative:



Another method involves the use of oxalyl chloride:

$$RCOOH + ClCOCOCl \rightarrow RCOCl + CO + CO_2 + HCl$$